



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:11 pm BST

PDB ID : 6Q2D
Title : Crystal structure of Methanobrevibacter smithii Dph2 in complex with Methanobrevibacter smithii elongation factor 2
Authors : Fenwick, M.K.; Dong, M.; Lin, H.; Ealick, S.E.
Deposited on : 2019-08-07
Resolution : 3.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

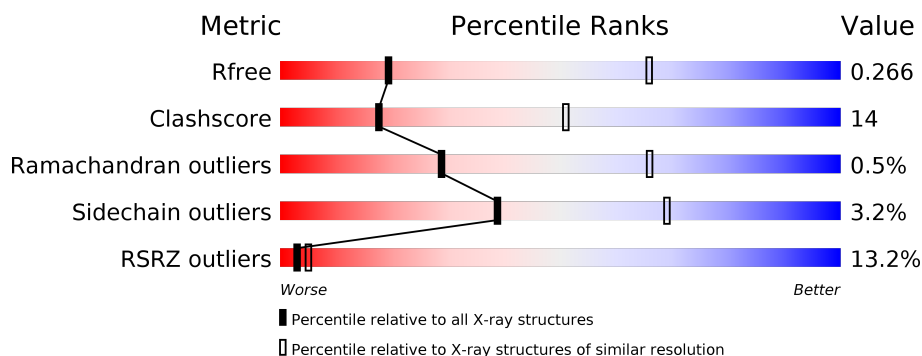
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	337	<div> <div>7%</div> <div>78%</div> <div>18%</div> <div>••</div> </div>
1	B	337	<div> <div>11%</div> <div>69%</div> <div>27%</div> <div>••</div> </div>
2	C	733	<div> <div>3%</div> <div>63%</div> <div>30%</div> <div>• 5%</div> </div>
2	F	733	<div> <div>19%</div> <div>41%</div> <div>56%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	A	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12185 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 2-(3-amino-3-carboxypropyl)histidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2586	1661	427	485	13			
1	B	325	Total	C	N	O	S	0	0	0
			2570	1652	423	482	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A5UMY5
A	-1	SER	-	expression tag	UNP A5UMY5
A	0	HIS	-	expression tag	UNP A5UMY5
B	-2	GLY	-	expression tag	UNP A5UMY5
B	-1	SER	-	expression tag	UNP A5UMY5
B	0	HIS	-	expression tag	UNP A5UMY5

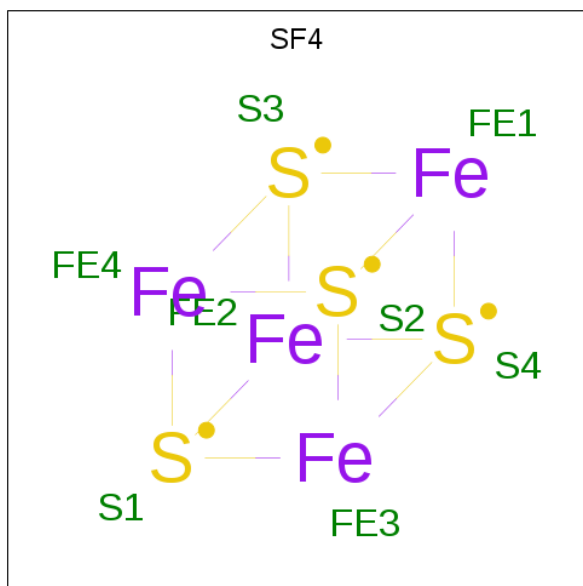
- Molecule 2 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	700	Total	C	N	O	S	0	0	0
			5406	3408	922	1046	30			
2	F	326	Total	C	N	O		0	0	0
			1607	955	326	326				

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A2H4U7K7
C	-1	SER	-	expression tag	UNP A0A2H4U7K7
C	0	GLY	-	expression tag	UNP A0A2H4U7K7
F	-2	GLY	-	expression tag	UNP A0A2H4U7K7
F	-1	SER	-	expression tag	UNP A0A2H4U7K7
F	0	GLY	-	expression tag	UNP A0A2H4U7K7

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

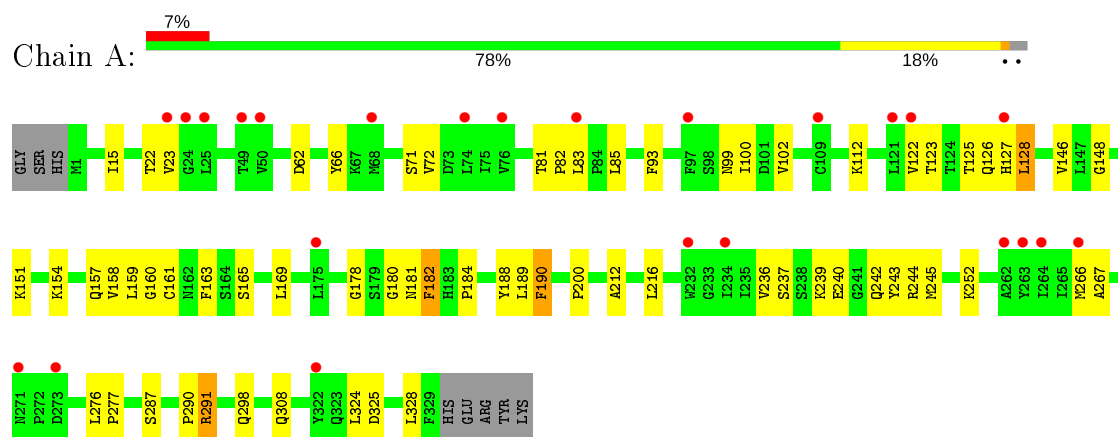


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	B	1	Total	Fe	S	0	0
			8	4	4		

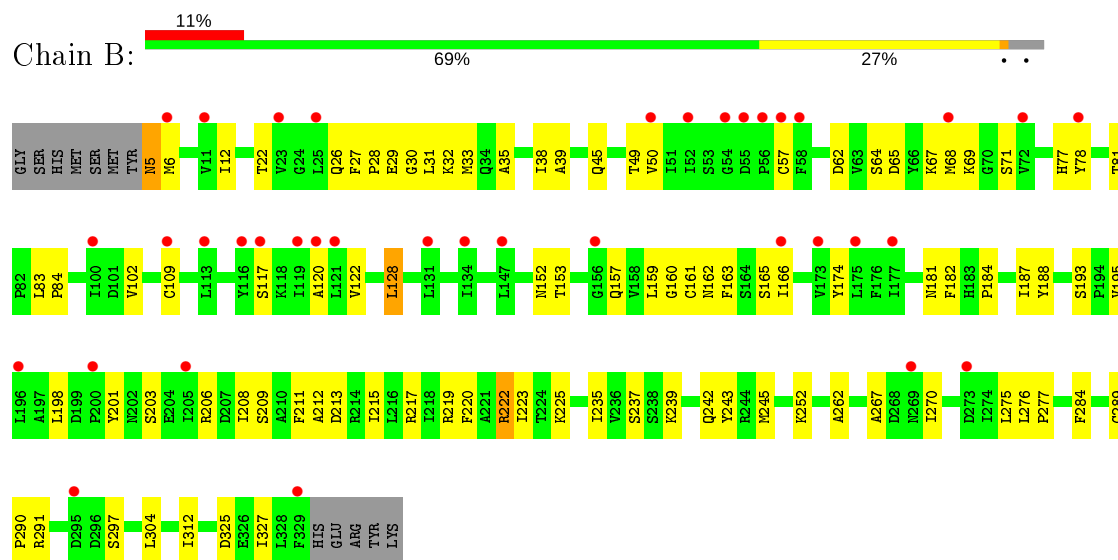
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 2-(3-amino-3-carboxypropyl)histidine synthase

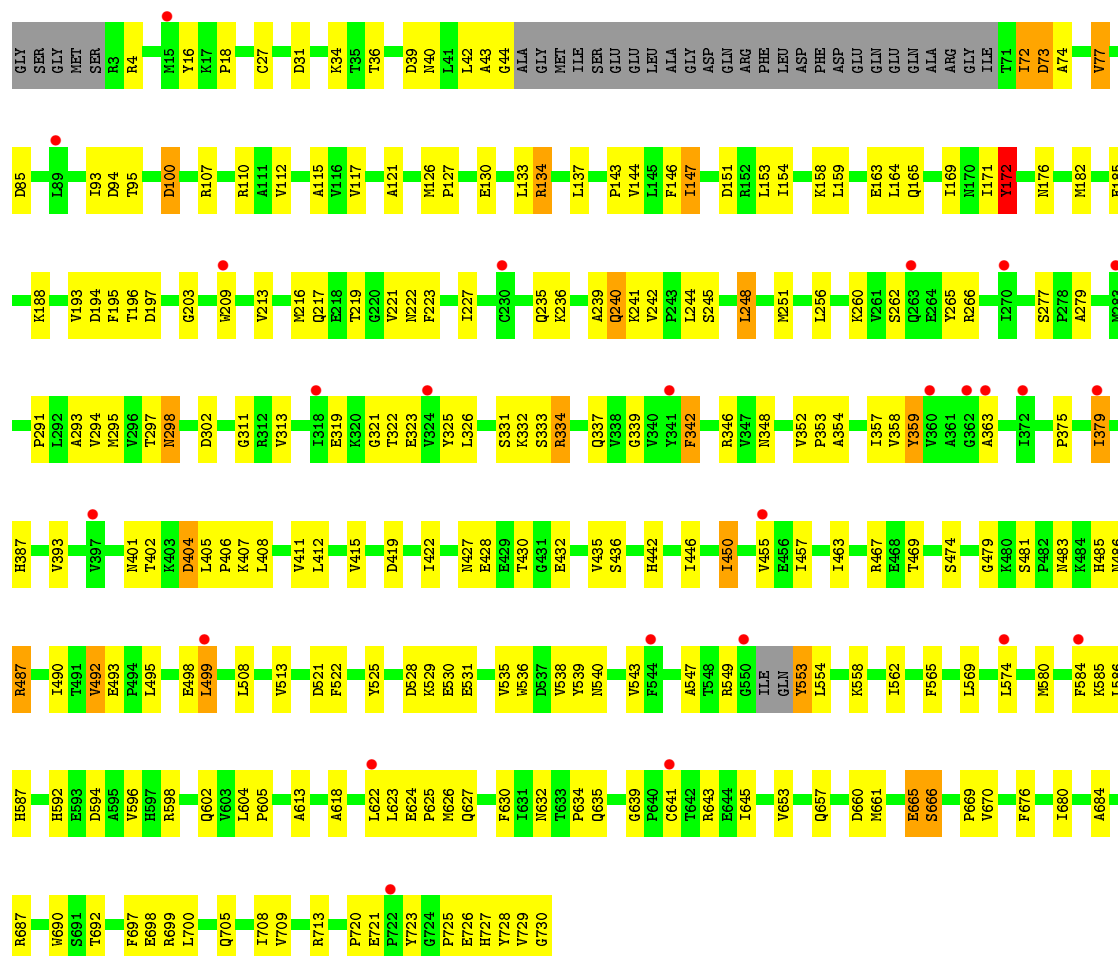


- Molecule 1: 2-(3-amino-3-carboxypropyl)histidine synthase

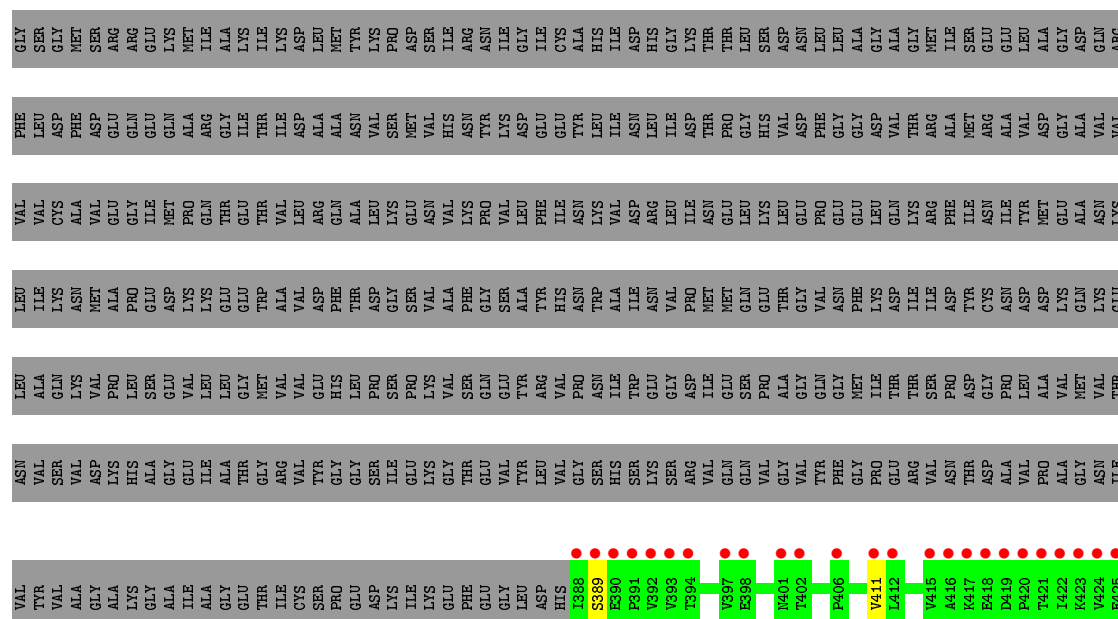
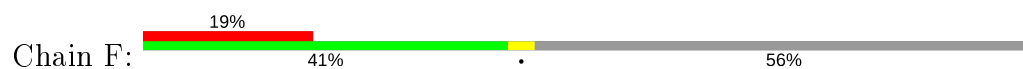


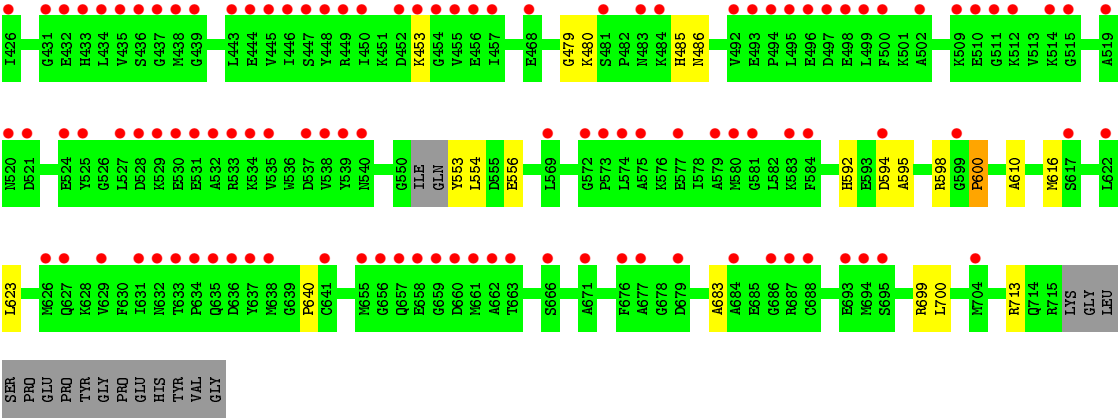
- Molecule 2: Elongation factor 2





• Molecule 2: Elongation factor 2





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	100.90Å 322.98Å 172.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 3.45 49.36 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.36-3.45) 99.6 (49.36-3.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.14_3211	Depositor
R, R_{free}	0.224 , 0.267 0.224 , 0.266	Depositor DCC
R_{free} test set	1869 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	139.3	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 189.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12185	wwPDB-VP
Average B, all atoms (Å ²)	208.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.43	0/2633	0.72	3/3561 (0.1%)
1	B	0.41	0/2617	0.67	0/3538
2	C	0.54	0/5502	0.84	3/7442 (0.0%)
2	F	0.51	0/1605	0.56	0/2230
All	All	0.49	0/12357	0.75	6/16771 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
2	C	0	4
2	F	0	1
All	All	0	8

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	172	TYR	CB-CA-C	7.42	125.24	110.40
1	A	182	PHE	N-CA-CB	7.04	123.27	110.60
1	A	291	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	A	291	ARG	NE-CZ-NH1	5.71	123.15	120.30
2	C	240	GLN	C-N-CA	-5.31	108.42	121.70
2	C	553	TYR	CB-CG-CD2	5.01	124.01	121.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	B	102	VAL	Peptide
1	B	5	ASN	Peptide
2	C	134	ARG	Sidechain
2	C	302	ASP	Peptide
2	C	4	ARG	Sidechain
2	C	486	ASN	Peptide
2	F	556	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2586	0	2617	59	0
1	B	2570	0	2606	70	0
2	C	5406	0	5367	189	1
2	F	1607	0	723	15	0
3	A	8	0	0	3	0
3	B	8	0	0	1	0
All	All	12185	0	11313	322	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ASN:OD1	1:B:206:ARG:NH2	1.97	0.96
2:F:640:PRO:CB	2:F:683:ALA:O	2.14	0.95
1:A:161:CYS:SG	3:A:401:SF4:FE2	1.63	0.91
1:B:211:PHE:CE2	1:B:215:ILE:HD11	2.13	0.83
1:B:225:LYS:HG2	2:C:428:GLU:OE2	1.79	0.82
2:C:159:LEU:HD22	2:C:163:GLU:HB3	1.65	0.78
2:C:313:VAL:HG23	2:C:358:VAL:CG2	2.14	0.77
2:C:467:ARG:HH11	2:C:580:MET:HB3	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:325:TYR:HD1	2:C:331:SER:O	1.70	0.75
2:C:626:MET:SD	2:C:698:GLU:HG3	2.27	0.75
1:A:146:VAL:HG21	1:A:169:LEU:HD22	1.68	0.75
1:A:161:CYS:HG	3:A:401:SF4:FE2	1.03	0.75
2:C:645:ILE:HD13	2:C:666:SER:OG	1.87	0.74
2:C:40:ASN:O	2:C:43:ALA:HB3	1.87	0.73
2:C:411:VAL:HG21	2:C:455:VAL:HG23	1.72	0.72
2:C:538:VAL:HG22	2:C:543:VAL:HG12	1.71	0.71
1:A:161:CYS:SG	3:A:401:SF4:S4	2.89	0.71
2:C:279:ALA:HA	2:C:291:PRO:HG2	1.74	0.70
2:C:513:VAL:HG21	2:C:535:VAL:HG13	1.74	0.70
2:C:262:SER:HA	2:C:265:TYR:CE2	2.27	0.69
2:C:346:ARG:HD2	2:C:359:TYR:CD2	2.28	0.69
2:C:450:ILE:HG21	2:C:457:ILE:CD1	2.23	0.69
2:C:337:GLN:NE2	2:C:348:ASN:HB3	2.07	0.69
2:C:342:PHE:O	2:C:342:PHE:HD2	1.76	0.68
1:B:161:CYS:SG	1:B:327:ILE:HB	2.33	0.68
2:C:154:ILE:HG23	2:C:227:ILE:HG23	1.75	0.67
2:C:408:LEU:HA	2:C:455:VAL:HG21	1.77	0.67
1:A:308:GLN:OE1	1:A:325:ASP:HB2	1.94	0.66
1:A:189:LEU:HD22	1:A:216:LEU:HD21	1.78	0.66
1:A:81:THR:HG21	1:A:154:LYS:HD2	1.78	0.66
2:C:130:GLU:O	2:C:134:ARG:HG3	1.97	0.65
1:A:102:VAL:HG12	1:A:200:PRO:HB3	1.79	0.65
1:B:290:PRO:HB3	1:B:325:ASP:HB3	1.78	0.65
1:A:163:PHE:HD1	1:A:190:PHE:CD2	2.15	0.64
1:B:211:PHE:CE2	1:B:215:ILE:CD1	2.81	0.63
2:C:16:TYR:CD1	2:C:353:PRO:HG3	2.33	0.63
1:B:211:PHE:CZ	1:B:215:ILE:HD11	2.33	0.63
1:B:5:ASN:OD1	1:B:6:MET:N	2.32	0.63
1:A:160:GLY:HA2	1:A:182:PHE:HE2	1.64	0.63
1:A:244:ARG:HD3	1:A:287:SER:O	1.98	0.63
2:C:34:LYS:NZ	2:C:95:THR:O	2.32	0.63
1:A:163:PHE:CD1	1:A:190:PHE:CD2	2.87	0.62
1:A:243:TYR:CZ	1:A:245:MET:HB2	2.35	0.62
2:C:467:ARG:NE	2:C:580:MET:SD	2.71	0.62
2:F:623:LEU:HA	2:F:700:LEU:H	1.64	0.62
2:C:492:VAL:CG1	2:C:584:PHE:CE2	2.84	0.61
2:C:531:GLU:OE2	2:C:585:LYS:HE2	2.01	0.61
1:A:82:PRO:HB3	1:A:93:PHE:CZ	2.36	0.60
2:C:467:ARG:HH11	2:C:580:MET:CB	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PHE:CB	1:A:291:ARG:HH21	2.15	0.60
2:C:553:TYR:O	2:C:554:LEU:HB2	2.02	0.60
1:B:12:ILE:HD13	1:B:45:GLN:OE1	2.03	0.59
2:C:337:GLN:HG2	2:C:348:ASN:HD22	1.67	0.59
2:C:342:PHE:CD2	2:C:342:PHE:O	2.55	0.59
2:C:485:HIS:HB3	2:C:592:HIS:CB	2.33	0.58
1:A:123:THR:HG23	1:A:128:LEU:HD13	1.85	0.58
2:C:450:ILE:HG21	2:C:457:ILE:HD13	1.86	0.58
1:A:163:PHE:HD1	1:A:190:PHE:CG	2.21	0.58
2:C:72:ILE:HD13	2:C:77:VAL:HG21	1.85	0.58
1:A:160:GLY:CA	1:A:182:PHE:HE2	2.17	0.58
1:B:122:VAL:HG22	1:B:166:ILE:HG21	1.86	0.58
1:A:123:THR:OG1	1:A:127:HIS:HB2	2.03	0.57
2:C:337:GLN:CG	2:C:348:ASN:HD22	2.18	0.57
1:B:81:THR:HG21	1:B:157:GLN:HE22	1.69	0.57
2:C:634:PRO:HG2	2:C:687:ARG:HD3	1.85	0.57
2:C:339:GLY:HA3	2:C:359:TYR:CE1	2.39	0.57
2:C:632:ASN:HB3	2:C:661:MET:CE	2.34	0.57
2:C:73:ASP:N	2:C:73:ASP:OD1	2.38	0.57
2:C:279:ALA:HA	2:C:291:PRO:CG	2.34	0.57
1:A:188:TYR:CD2	1:A:212:ALA:CB	2.88	0.56
1:B:219:ARG:HH12	1:B:297:SER:CB	2.17	0.56
2:C:574:LEU:HD21	2:C:705:GLN:NE2	2.19	0.56
2:C:325:TYR:HB3	2:C:375:PRO:HA	1.86	0.56
1:B:120:ALA:HB3	1:B:174:TYR:CD1	2.41	0.56
2:C:508:LEU:HD21	2:C:521:ASP:HB3	1.87	0.56
2:C:144:VAL:HG23	2:C:256:LEU:HD21	1.88	0.55
1:A:82:PRO:HB3	1:A:93:PHE:CE2	2.42	0.55
2:C:558:LYS:O	2:C:562:ILE:HG12	2.06	0.55
2:C:613:ALA:HB2	2:C:728:TYR:CB	2.35	0.55
1:B:160:GLY:O	1:B:182:PHE:HE2	1.90	0.55
2:C:159:LEU:HD12	2:C:164:LEU:HD12	1.88	0.55
2:C:339:GLY:HA3	2:C:359:TYR:HE1	1.70	0.55
1:A:244:ARG:HH12	1:A:325:ASP:CG	2.09	0.55
1:B:239:LYS:HD2	1:B:242:GLN:NE2	2.22	0.55
2:C:334:ARG:HG3	2:C:334:ARG:NH2	2.22	0.55
2:C:159:LEU:HB2	2:C:164:LEU:HD12	1.89	0.54
1:B:213:ASP:O	1:B:217:ARG:HG3	2.08	0.54
2:C:100:ASP:HB3	2:C:690:TRP:HE1	1.73	0.54
2:C:540:ASN:O	2:C:580:MET:HA	2.07	0.54
1:B:284:PHE:HB2	1:B:304:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:134:ARG:HE	2:C:182:MET:HE2	1.72	0.53
2:C:293:ALA:HA	2:C:379:ILE:HD13	1.90	0.53
2:C:479:GLY:O	2:C:487:ARG:HA	2.08	0.53
2:C:185:GLU:OE1	2:C:188:LYS:CE	2.56	0.53
1:B:26:GLN:OE1	1:B:77:HIS:ND1	2.40	0.53
2:C:313:VAL:HG23	2:C:358:VAL:HG21	1.89	0.53
2:C:352:VAL:HG11	2:C:358:VAL:HG22	1.91	0.53
1:A:125:THR:OG1	1:A:157:GLN:NE2	2.42	0.53
2:C:401:ASN:O	2:C:404:ASP:OD2	2.26	0.53
2:C:639:GLY:O	2:C:643:ARG:HG3	2.09	0.53
1:B:222:ARG:NH2	1:B:297:SER:HB2	2.23	0.53
2:C:107:ARG:HA	2:C:110:ARG:HD3	1.90	0.53
2:C:121:ALA:HB2	2:C:147:ILE:HG22	1.90	0.53
2:C:490:ILE:HG22	2:C:586:LEU:HA	1.89	0.52
2:C:547:ALA:HB3	2:C:587:HIS:HA	1.91	0.52
1:B:29:GLU:HG2	1:B:32:LYS:HE2	1.90	0.52
2:C:18:PRO:HB2	2:C:260:LYS:HB2	1.92	0.52
2:C:522:PHE:CZ	2:C:535:VAL:HG11	2.43	0.52
2:C:422:ILE:HD11	2:C:435:VAL:HG12	1.91	0.52
2:C:481:SER:OG	2:C:483:ASN:OD1	2.28	0.52
2:C:565:PHE:CE1	2:C:569:LEU:HD11	2.45	0.52
1:A:125:THR:HA	1:A:128:LEU:HD22	1.91	0.52
1:A:126:GLN:NE2	2:C:596:VAL:HG11	2.24	0.52
1:A:99:ASN:O	1:A:100:ILE:HD13	2.09	0.52
2:F:623:LEU:HA	2:F:700:LEU:N	2.25	0.52
1:A:182:PHE:HB2	1:A:291:ARG:HH21	1.75	0.52
1:B:276:LEU:N	1:B:277:PRO:HD2	2.25	0.51
1:B:327:ILE:HD12	3:B:401:SF4:S4	2.50	0.51
2:C:528:ASP:OD1	2:C:529:LYS:N	2.44	0.51
2:C:195:PHE:CE1	2:C:213:VAL:HG23	2.45	0.51
1:A:276:LEU:HB3	2:F:600:PRO:CB	2.41	0.51
1:B:188:TYR:CE2	1:B:209:SER:HA	2.46	0.51
2:C:321:GLY:HA2	2:C:334:ARG:HH11	1.76	0.51
2:C:332:LYS:HG2	2:C:333:SER:N	2.26	0.51
1:A:188:TYR:CD2	1:A:212:ALA:HB1	2.46	0.51
1:B:109:CYS:SG	1:B:198:LEU:HD22	2.51	0.51
1:B:38:ILE:HD13	1:B:78:TYR:OH	2.11	0.51
2:C:627:GLN:HG3	2:C:670:VAL:HG22	1.93	0.50
1:A:182:PHE:CE1	1:A:291:ARG:HG3	2.46	0.50
2:C:16:TYR:CE1	2:C:353:PRO:HG3	2.46	0.50
2:C:213:VAL:HA	2:C:216:MET:CE	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:TYR:HE2	1:A:240:GLU:OE1	1.93	0.50
1:B:239:LYS:HD2	1:B:242:GLN:HE21	1.76	0.50
1:B:222:ARG:HH21	1:B:297:SER:HB2	1.76	0.50
2:C:93:ILE:HD11	2:C:357:ILE:HG13	1.94	0.50
2:C:154:ILE:CG2	2:C:227:ILE:HG23	2.39	0.50
2:C:720:PRO:HB2	2:C:721:GLU:OE1	2.12	0.50
2:C:236:LYS:O	2:C:240:GLN:HG2	2.12	0.50
2:C:723:TYR:HD1	2:C:727:HIS:CD2	2.30	0.50
1:B:161:CYS:SG	1:B:327:ILE:HD12	2.52	0.49
1:B:212:ALA:O	1:B:213:ASP:C	2.51	0.49
1:A:123:THR:HG21	1:A:128:LEU:HA	1.95	0.49
2:C:151:ASP:HB3	2:C:235:GLN:OE1	2.13	0.49
2:F:480:LYS:HA	2:F:486:ASN:O	2.13	0.49
2:C:547:ALA:HB3	2:C:586:LEU:O	2.12	0.49
1:A:252:LYS:HE2	1:B:49:THR:HG23	1.95	0.49
2:C:625:PRO:HB3	2:C:697:PHE:CE1	2.47	0.49
1:A:298:GLN:NE2	2:C:483:ASN:O	2.43	0.49
2:C:492:VAL:CG1	2:C:584:PHE:CD2	2.95	0.49
1:A:290:PRO:HB3	1:A:325:ASP:HB3	1.95	0.48
1:A:276:LEU:N	1:A:277:PRO:CD	2.76	0.48
2:C:294:VAL:HG23	2:C:295:MET:N	2.28	0.48
2:C:223:PHE:O	2:C:227:ILE:HG13	2.13	0.48
1:B:217:ARG:NH1	2:C:402:THR:HG23	2.29	0.48
2:C:313:VAL:CG2	2:C:358:VAL:HG21	2.43	0.48
1:B:219:ARG:HH12	1:B:297:SER:HB2	1.79	0.48
2:C:219:THR:OG1	2:C:221:VAL:HG23	2.13	0.48
2:C:474:SER:HB3	2:C:618:ALA:HB2	1.95	0.48
2:C:632:ASN:HB3	2:C:661:MET:HE1	1.94	0.48
2:C:729:VAL:HG12	2:C:730:GLY:N	2.27	0.48
2:C:326:LEU:HD21	2:C:363:ALA:O	2.14	0.48
2:C:700:LEU:HD21	2:C:708:ILE:HD12	1.95	0.48
1:B:184:PRO:HA	1:B:187:ILE:HD12	1.96	0.48
2:C:147:ILE:HD13	2:C:171:ILE:HG21	1.96	0.48
2:C:598:ARG:HA	2:C:602:GLN:OE1	2.13	0.48
1:A:182:PHE:CB	1:A:291:ARG:NH2	2.76	0.47
2:C:334:ARG:HG3	2:C:334:ARG:HH21	1.79	0.47
2:C:635:GLN:OE1	2:C:657:GLN:NE2	2.47	0.47
2:C:44:GLY:HA3	2:C:245:SER:OG	2.14	0.47
2:C:159:LEU:HB2	2:C:164:LEU:CD1	2.43	0.47
2:C:422:ILE:HD12	2:C:436:SER:O	2.13	0.47
1:B:237:SER:HA	1:B:267:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:27:CYS:SG	2:C:115:ALA:HB1	2.55	0.47
2:C:415:VAL:HG11	2:C:446:ILE:HG23	1.97	0.47
1:A:237:SER:HA	1:A:267:ALA:O	2.13	0.47
1:A:62:ASP:OD1	1:A:239:LYS:HG2	2.15	0.47
1:B:152:ASN:HB2	1:B:162:ASN:HD21	1.79	0.47
2:C:203:GLY:HA2	2:C:209:TRP:CZ3	2.49	0.47
2:C:522:PHE:CE2	2:C:535:VAL:HG11	2.49	0.47
1:A:148:GLY:CA	1:A:169:LEU:HD11	2.45	0.47
2:C:313:VAL:CG1	2:C:354:ALA:HA	2.45	0.47
2:C:427:ASN:ND2	2:C:430:THR:OG1	2.48	0.46
2:C:553:TYR:O	2:C:554:LEU:CB	2.63	0.46
2:C:531:GLU:OE2	2:C:585:LYS:CE	2.63	0.46
2:F:411:VAL:CB	2:F:453:LYS:CB	2.93	0.46
1:B:153:THR:OG1	1:B:165:SER:HB3	2.14	0.46
1:B:181:ASN:HA	1:B:184:PRO:CG	2.46	0.46
1:B:276:LEU:N	1:B:277:PRO:CD	2.79	0.46
2:C:297:THR:HG23	2:C:311:GLY:HA2	1.96	0.46
1:A:236:VAL:O	1:A:266:MET:HA	2.16	0.46
2:C:407:LYS:O	2:C:411:VAL:HG23	2.15	0.46
2:C:169:ILE:HA	2:C:172:TYR:CD2	2.51	0.46
2:C:622:LEU:HD22	2:C:709:VAL:HG22	1.97	0.46
1:A:15:ILE:HG12	1:A:23:VAL:HG21	1.98	0.45
2:C:100:ASP:HB3	2:C:690:TRP:NE1	2.32	0.45
1:A:148:GLY:HA3	1:A:165:SER:O	2.16	0.45
2:C:185:GLU:OE1	2:C:188:LYS:HE2	2.17	0.45
1:B:225:LYS:CG	2:C:428:GLU:OE2	2.56	0.45
1:B:223:ILE:HG21	1:B:312:ILE:HG22	1.98	0.45
1:B:57:CYS:HA	1:B:62:ASP:OD2	2.16	0.45
2:C:154:ILE:HD13	2:C:227:ILE:HA	1.97	0.45
2:C:194:ASP:OD1	2:C:196:THR:HB	2.16	0.45
2:C:319:GLU:HB2	2:C:322:THR:OG1	2.17	0.45
2:C:326:LEU:CD1	2:C:326:LEU:N	2.79	0.45
1:B:220:PHE:HA	1:B:223:ILE:HD12	1.98	0.45
2:C:172:TYR:CE2	2:C:195:PHE:HB2	2.52	0.45
2:C:624:GLU:N	2:C:698:GLU:O	2.50	0.45
1:B:81:THR:CG2	1:B:157:GLN:HE22	2.28	0.45
2:C:342:PHE:CD2	2:C:342:PHE:C	2.90	0.45
2:C:492:VAL:HG11	2:C:584:PHE:CE2	2.52	0.45
2:C:334:ARG:HH21	2:C:334:ARG:CG	2.30	0.45
1:A:112:LYS:HD2	1:A:112:LYS:HA	1.70	0.45
1:B:128:LEU:HD11	1:B:157:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:393:VAL:HG13	2:C:463:ILE:O	2.17	0.45
2:C:676:PHE:CZ	2:C:680:ILE:HD12	2.52	0.45
1:A:188:TYR:HD2	1:A:212:ALA:HB1	1.82	0.44
1:B:83:LEU:HB3	1:B:84:PRO:HD2	1.99	0.44
2:C:419:ASP:O	2:C:422:ILE:HG22	2.17	0.44
2:C:690:TRP:HZ3	2:C:692:THR:HG23	1.82	0.44
2:C:721:GLU:OE2	2:F:616:MET:O	2.34	0.44
2:C:74:ALA:O	2:C:94:ASP:HB2	2.17	0.44
1:B:27:PHE:CE2	1:B:35:ALA:HB2	2.52	0.44
2:C:134:ARG:HE	2:C:182:MET:CE	2.30	0.44
2:C:159:LEU:HB3	2:C:163:GLU:HB2	1.98	0.44
2:C:498:GLU:HB2	2:C:525:TYR:O	2.17	0.44
1:A:146:VAL:CG2	1:A:169:LEU:HD22	2.44	0.44
2:C:405:LEU:HB3	2:C:406:PRO:HD3	2.00	0.44
1:B:22:THR:HG21	1:B:71:SER:O	2.17	0.44
2:C:126:MET:HB3	2:C:127:PRO:HD2	1.99	0.44
2:C:213:VAL:HA	2:C:216:MET:HE2	2.00	0.44
2:C:411:VAL:HG21	2:C:455:VAL:CG2	2.45	0.44
2:C:604:LEU:N	2:C:605:PRO:HD2	2.31	0.44
2:C:469:THR:HG22	2:C:623:LEU:HD11	1.99	0.44
2:F:485:HIS:O	2:F:592:HIS:CB	2.66	0.44
1:A:22:THR:HG22	1:A:72:VAL:HA	2.00	0.44
2:C:112:VAL:O	2:C:266:ARG:CZ	2.66	0.44
1:A:180:GLY:O	1:A:184:PRO:HD2	2.17	0.44
1:A:236:VAL:HA	1:A:287:SER:HG	1.83	0.44
1:B:28:PRO:HD2	1:B:31:LEU:HD12	2.00	0.44
1:B:235:ILE:HG21	1:B:270:ILE:HG12	2.00	0.44
2:C:248:LEU:HG	2:C:251:MET:HE1	2.00	0.44
1:A:181:ASN:O	1:A:182:PHE:C	2.55	0.43
2:C:137:LEU:HD21	2:C:143:PRO:HG3	1.99	0.43
2:C:159:LEU:CD1	2:C:164:LEU:HD12	2.46	0.43
2:C:528:ASP:HB3	2:C:531:GLU:HG3	1.99	0.43
2:C:626:MET:HG2	2:C:669:PRO:HA	2.00	0.43
2:C:72:ILE:HG22	2:C:73:ASP:N	2.32	0.43
1:B:223:ILE:HG21	1:B:312:ILE:CG2	2.48	0.43
2:C:705:GLN:O	2:C:709:VAL:HG23	2.19	0.43
2:C:144:VAL:HG23	2:C:256:LEU:CD2	2.47	0.43
2:F:479:GLY:HA3	2:F:610:ALA:HB2	1.99	0.43
1:A:122:VAL:CG1	1:A:158:VAL:HG13	2.48	0.43
1:A:83:LEU:HB3	1:A:85:LEU:HG	2.01	0.43
1:B:289:CYS:SG	1:B:291:ARG:HB2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:134:ARG:NH2	2:C:634:PRO:HG3	2.34	0.43
1:B:39:ALA:HA	1:B:50:VAL:HG21	2.00	0.43
2:C:93:ILE:HD11	2:C:357:ILE:CG1	2.49	0.43
2:C:630:PHE:O	2:C:690:TRP:HB2	2.19	0.43
1:B:208:ILE:HA	1:B:208:ILE:HD12	1.85	0.43
2:C:146:PHE:CD2	2:C:248:LEU:HD11	2.53	0.43
1:B:159:LEU:HB2	1:B:162:ASN:HB3	2.00	0.43
1:B:290:PRO:CB	1:B:325:ASP:HB3	2.46	0.43
1:A:159:LEU:O	1:A:163:PHE:CE2	2.72	0.42
2:C:209:TRP:HB3	2:C:239:ALA:HA	2.01	0.42
2:C:613:ALA:HB2	2:C:728:TYR:HB2	2.00	0.42
1:A:239:LYS:HB2	1:A:242:GLN:HB2	2.00	0.42
2:C:485:HIS:HB3	2:C:592:HIS:HB2	2.01	0.42
2:C:726:GLU:HG2	2:F:713:ARG:CB	2.49	0.42
1:B:184:PRO:HB2	1:B:208:ILE:HG12	2.00	0.42
2:C:323:GLU:HG3	2:C:334:ARG:HB2	2.02	0.42
1:B:160:GLY:O	1:B:163:PHE:HE2	2.02	0.42
2:C:165:GLN:OE1	2:C:223:PHE:CZ	2.72	0.42
2:C:93:ILE:HD11	2:C:357:ILE:HD11	1.99	0.42
1:B:30:GLY:HA2	2:F:598:ARG:O	2.19	0.42
2:C:39:ASP:O	2:C:42:LEU:HB3	2.20	0.42
2:C:641:CYS:SG	2:C:684:ALA:HB2	2.59	0.42
1:A:243:TYR:CZ	1:A:245:MET:CB	3.01	0.42
1:B:252:LYS:NZ	1:B:262:ALA:O	2.53	0.42
1:B:161:CYS:HB3	1:B:290:PRO:HG2	2.02	0.42
1:B:5:ASN:OD1	1:B:5:ASN:C	2.58	0.42
1:A:163:PHE:CE1	1:A:324:LEU:HD12	2.55	0.42
2:C:574:LEU:O	2:C:713:ARG:HD2	2.20	0.42
2:C:222:ASN:OD1	2:C:222:ASN:C	2.59	0.42
2:C:405:LEU:HD12	2:C:405:LEU:HA	1.87	0.42
2:C:298:ASN:C	2:C:298:ASN:OD1	2.57	0.41
1:A:81:THR:HG21	1:A:154:LYS:CD	2.49	0.41
2:C:121:ALA:HB1	2:C:153:LEU:HD11	2.02	0.41
2:C:635:GLN:HG2	2:C:660:ASP:O	2.21	0.41
2:F:623:LEU:HA	2:F:699:ARG:HA	2.02	0.41
1:A:148:GLY:HA3	1:A:169:LEU:HD11	2.02	0.41
2:C:134:ARG:HH11	2:C:182:MET:HE2	1.85	0.41
2:C:194:ASP:HB3	2:C:197:ASP:OD1	2.20	0.41
2:C:412:LEU:HD23	2:C:450:ILE:HD11	2.02	0.41
2:C:495:LEU:HD11	2:C:499:LEU:HD13	2.02	0.41
1:B:201:TYR:CE1	2:F:595:ALA:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ASP:O	1:B:69:LYS:HB2	2.20	0.41
2:C:134:ARG:NE	2:C:182:MET:CE	2.84	0.41
2:C:159:LEU:HD22	2:C:163:GLU:CB	2.45	0.41
2:C:405:LEU:CB	2:C:406:PRO:HD3	2.50	0.41
2:C:530:GLU:OE1	2:C:549:ARG:NH2	2.53	0.41
2:C:725:PRO:O	2:C:729:VAL:HG23	2.21	0.41
2:C:729:VAL:CG1	2:C:730:GLY:N	2.83	0.41
1:B:243:TYR:CZ	1:B:245:MET:HB2	2.55	0.41
2:F:485:HIS:O	2:F:592:HIS:N	2.49	0.41
1:A:239:LYS:HD2	1:A:242:GLN:CD	2.42	0.41
1:B:290:PRO:HG3	1:B:325:ASP:CG	2.41	0.41
1:B:64:SER:HB2	1:B:67:LYS:HB2	2.03	0.41
2:C:244:LEU:O	2:C:248:LEU:HB2	2.21	0.41
1:B:193:SER:O	1:B:195:VAL:HG23	2.21	0.41
2:C:430:THR:HG21	2:C:432:GLU:OE1	2.21	0.41
2:F:553:TYR:O	2:F:554:LEU:CB	2.68	0.41
1:B:195:VAL:HB	1:B:208:ILE:HG22	2.03	0.40
1:B:275:LEU:HD22	1:B:284:PHE:CE1	2.56	0.40
2:C:411:VAL:O	2:C:415:VAL:HG23	2.21	0.40
2:C:44:GLY:HA3	2:C:245:SER:CB	2.52	0.40
2:C:623:LEU:HA	2:C:699:ARG:HA	2.03	0.40
2:C:653:VAL:HB	2:C:665:GLU:HB3	2.03	0.40
1:B:128:LEU:HD12	1:B:128:LEU:HA	1.96	0.40
2:C:117:VAL:HG21	2:C:133:LEU:HD13	2.02	0.40
2:C:442:HIS:O	2:C:446:ILE:HG12	2.21	0.40
2:C:176:ASN:OD1	2:C:193:VAL:HG22	2.22	0.40
2:C:93:ILE:HD11	2:C:357:ILE:CD1	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:GLN:OE1	2:C:217:GLN:OE1[3_655]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/337 (97%)	315 (96%)	12 (4%)	0	100	100
1	B	323/337 (96%)	310 (96%)	13 (4%)	0	100	100
2	C	694/733 (95%)	665 (96%)	24 (4%)	5 (1%)	22	60
2	F	322/733 (44%)	310 (96%)	9 (3%)	3 (1%)	17	54
All	All	1666/2140 (78%)	1600 (96%)	58 (4%)	8 (0%)	29	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	600	PRO
2	C	487	ARG
2	C	158	LYS
2	F	389	SER
2	C	387	HIS
2	C	539	TYR
2	F	594	ASP
2	C	72	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/299 (94%)	277 (98%)	5 (2%)	59	81
1	B	282/299 (94%)	276 (98%)	6 (2%)	53	78
2	C	583/621 (94%)	557 (96%)	26 (4%)	27	60
All	All	1147/1219 (94%)	1110 (97%)	37 (3%)	39	69

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	128	LEU
1	A	151	LYS
1	A	190	PHE
1	A	328	LEU
1	B	33	MET
1	B	68	MET
1	B	117	SER
1	B	128	LEU
1	B	203	SER
1	B	222	ARG
2	C	31	ASP
2	C	36	THR
2	C	73	ASP
2	C	77	VAL
2	C	85	ASP
2	C	100	ASP
2	C	147	ILE
2	C	172	TYR
2	C	241	LYS
2	C	242	VAL
2	C	248	LEU
2	C	277	SER
2	C	298	ASN
2	C	334	ARG
2	C	342	PHE
2	C	359	TYR
2	C	379	ILE
2	C	404	ASP
2	C	450	ILE
2	C	492	VAL
2	C	493	GLU
2	C	499	LEU
2	C	536	TRP
2	C	594	ASP
2	C	665	GLU
2	C	666	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	GLN
1	A	269	ASN

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Mol	Chain	Res	Type
1	B	157	GLN
2	C	208	ASN
2	C	348	ASN
2	C	427	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SF4	B	401	1	0,12,12	0.00	-	-		
3	SF4	A	401	1	0,12,12	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SF4	B	401	1	-	-	0/6/5/5
3	SF4	A	401	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	SF4	1	0
3	A	401	SF4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	329/337 (97%)	0.47	24 (7%) 15 17	134, 205, 255, 285	0
1	B	325/337 (96%)	0.59	37 (11%) 5 7	124, 231, 302, 328	0
2	C	700/733 (95%)	0.27	25 (3%) 42 41	87, 157, 218, 267	0
2	F	326/733 (44%)	2.24	136 (41%) 0 0	275, 339, 391, 425	0
All	All	1680/2140 (78%)	0.75	222 (13%) 3 5	87, 196, 361, 425	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	424	VAL	11.0
2	F	531	GLU	10.7
2	F	530	GLU	10.7
2	F	392	VAL	10.5
2	F	539	TYR	9.0
2	F	634	PRO	8.6
2	F	529	LYS	8.6
2	F	425	GLU	8.5
2	F	493	GLU	8.4
2	F	532	ALA	8.4
2	F	416	ALA	8.2
2	F	455	VAL	8.1
2	F	421	THR	7.8
2	F	573	PRO	7.7
2	F	494	PRO	7.7
2	F	574	LEU	7.5
2	F	433	HIS	7.4
2	F	422	ILE	7.3
2	F	688	CYS	7.3
2	F	533	ARG	7.0
2	F	438	MET	6.9

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Mol	Chain	Res	Type	RSRZ
2	F	391	PRO	6.9
2	F	446	ILE	6.7
2	F	635	GLN	6.7
2	F	447	SER	6.6
2	F	528	ASP	6.5
2	F	437	GLY	6.5
2	F	419	ASP	6.2
2	F	633	THR	6.2
2	F	660	ASP	6.2
1	B	121	LEU	6.2
2	F	659	GLY	6.1
2	F	397	VAL	6.1
2	F	510	GLU	6.0
2	F	538	VAL	5.9
2	F	638	MET	5.7
2	F	636	ASP	5.6
2	F	498	GLU	5.5
2	F	499	LEU	5.5
2	F	426	ILE	5.5
2	F	434	LEU	5.4
2	F	420	PRO	5.3
2	F	534	LYS	5.2
2	F	435	VAL	5.2
1	B	119	ILE	5.1
2	F	393	VAL	5.1
2	F	521	ASP	5.1
2	F	452	ASP	5.0
2	F	449	ARG	5.0
2	F	694	MET	5.0
2	C	550	GLY	4.9
1	B	200	PRO	4.8
2	F	436	SER	4.8
2	F	453	LYS	4.8
2	F	415	VAL	4.8
2	F	525	TYR	4.8
1	B	205	ILE	4.8
2	F	394	THR	4.7
2	F	637	TYR	4.6
2	F	454	GLY	4.6
2	F	492	VAL	4.6
2	F	401	ASN	4.6
2	F	656	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
2	F	579	ALA	4.5
2	F	657	GLN	4.4
1	B	6	MET	4.4
2	F	569	LEU	4.4
2	F	575	ALA	4.3
1	B	25	LEU	4.3
2	F	418	GLU	4.3
2	C	283	MET	4.3
2	F	695	SER	4.2
2	F	632	ASN	4.1
2	F	524	GLU	4.1
2	F	661	MET	4.0
1	A	322	TYR	4.0
2	F	412	LEU	3.9
2	F	658	GLU	3.9
2	F	417	LYS	3.8
2	F	666	SER	3.8
2	F	540	ASN	3.8
2	F	622	LEU	3.8
1	A	262	ALA	3.7
2	F	443	LEU	3.7
2	F	663	THR	3.7
1	B	109	CYS	3.7
1	A	263	TYR	3.7
2	F	468	GLU	3.7
1	B	55	ASP	3.7
1	A	273	ASP	3.6
2	F	423	LYS	3.6
2	F	583	LYS	3.6
2	F	627	GLN	3.5
1	A	50	VAL	3.5
2	F	497	ASP	3.5
2	F	511	GLY	3.5
2	F	390	GLU	3.5
2	F	572	GLY	3.5
1	B	57	CYS	3.5
1	B	50	VAL	3.4
1	B	78	TYR	3.4
2	F	500	PHE	3.4
1	A	127	HIS	3.3
1	A	234	ILE	3.3
2	F	520	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	448	TYR	3.3
1	A	175	LEU	3.3
1	B	72	VAL	3.3
2	F	389	SER	3.2
1	B	173	VAL	3.2
2	F	445	VAL	3.2
1	B	116	TYR	3.2
2	C	574	LEU	3.2
2	F	388	ILE	3.2
1	A	25	LEU	3.2
2	F	580	MET	3.2
2	C	379	ILE	3.1
2	C	360	VAL	3.1
2	F	662	ALA	3.1
2	F	439	GLY	3.1
2	F	527	LEU	3.1
1	B	58	PHE	3.1
2	C	230	CYS	3.0
1	A	76	VAL	3.0
2	F	686	GLY	3.0
2	C	722	PRO	3.0
1	B	11	VAL	3.0
2	F	431	GLY	3.0
2	C	372	ILE	3.0
2	F	411	VAL	3.0
2	F	495	LEU	2.9
1	A	266	MET	2.9
2	C	363	ALA	2.9
2	F	432	GLU	2.9
2	F	514	LYS	2.9
2	F	617	SER	2.9
2	F	456	GLU	2.9
1	A	24	GLY	2.9
2	F	450	ILE	2.9
2	C	362	GLY	2.9
1	A	23	VAL	2.8
2	F	457	ILE	2.8
1	A	122	VAL	2.8
1	B	56	PRO	2.8
2	F	655	MET	2.8
2	F	594	ASP	2.8
2	F	496	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	687	ARG	2.8
2	F	671	ALA	2.8
2	F	406	PRO	2.7
2	F	515	GLY	2.7
2	F	519	ALA	2.7
2	C	641	CYS	2.7
2	F	641	CYS	2.7
2	F	509	LYS	2.6
1	A	109	CYS	2.6
1	A	271	ASN	2.6
1	A	49	THR	2.6
2	F	402	THR	2.5
2	F	684	ALA	2.5
1	B	54	GLY	2.5
1	B	147	LEU	2.5
1	B	177	ILE	2.5
2	F	444	GLU	2.5
2	C	499	LEU	2.5
1	B	196	LEU	2.5
2	C	15	MET	2.5
2	F	584	PHE	2.5
2	F	577	GLU	2.5
1	A	74	LEU	2.5
1	B	134	ILE	2.5
2	F	398	GLU	2.4
2	C	544	PHE	2.4
1	B	329	PHE	2.4
1	B	23	VAL	2.4
1	B	120	ALA	2.4
1	B	156	GLY	2.4
2	F	535	VAL	2.3
2	F	581	GLY	2.3
2	F	676	PHE	2.3
2	F	677	ALA	2.3
2	F	629	VAL	2.3
2	F	693	GLU	2.3
1	A	68	MET	2.3
2	F	537	ASP	2.3
2	F	481	SER	2.3
1	B	175	LEU	2.3
1	B	273	ASP	2.3
2	F	484	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	324	VAL	2.3
1	B	68	MET	2.2
2	C	318	ILE	2.2
2	F	512	LYS	2.2
1	A	264	ILE	2.2
2	C	263	GLN	2.2
1	B	117	SER	2.2
2	F	631	ILE	2.2
2	C	89	LEU	2.2
1	B	269	ASN	2.2
2	F	483	ASN	2.2
1	B	52	ILE	2.2
1	A	121	LEU	2.2
2	C	209	TRP	2.1
1	B	166	ILE	2.1
1	B	113	LEU	2.1
2	F	679	ASP	2.1
1	A	232	TRP	2.1
2	F	502	ALA	2.1
2	F	626	MET	2.1
1	B	131	LEU	2.1
2	C	622	LEU	2.1
2	F	704	MET	2.1
1	A	97	PHE	2.1
1	B	100	ILE	2.1
2	C	341	TYR	2.0
2	C	455	VAL	2.0
2	C	270	ILE	2.0
2	C	397	VAL	2.0
1	B	295	ASP	2.0
1	A	83	LEU	2.0
2	C	584	PHE	2.0
2	F	599	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SF4	A	401	8/8	0.98	0.27	154,168,236,240	0
3	SF4	B	401	8/8	0.99	0.27	164,225,278,279	0

6.5 Other polymers [i](#)

There are no such residues in this entry.